Control Volume Hydrodynamics (CVH) Package Users' Guide

The Control Volume Hydrodynamics (CVH) and Flow Path (FL) packages are responsible for modeling the thermal-hydraulic behavior of liquid water, water vapor, and gases in MELCOR. Modeling is based on a control volume/flow path formulation and is described in detail in the Thermal Hydraulic (CVH and FL) Package's Reference Manual.

This Users' Guide describes input to the CVH package, which is concerned with the geometry and contents of control volumes. CVH input describes the initial state of each volume; optional input allows the definition of sources and sinks of mass and/or energy, in terms of data from the Control Function (CF) and Tabular Function (TF) packages. Additional sources and sinks may be imposed by other packages during a MELCOR calculation; these are treated automatically and do not require input to CVH. Similarly, changes in control volume geometry resulting from relocation of nonhydrodynamic materials is communicated to CVH during MELCOR execution; no CVH input is required.

Connections *between* control volumes, through which the control volume contents may flow, are defined by input to the Flow Path package, which is described in the FL Package Users' Guide.

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1. Control Volume Models

All hydrodynamic material, together with its associated energy, in a MELCOR calculation resides in *control volumes*. Hydrodynamic material includes the coolant (water), vapor and fog, and noncondensible gases; it does not include core structures or core debris, other heat structures, fission products, aerosols, water films on heat structures or ice in ice condensers.

1.1 Control Volume Geometry

The spatial geometry of a control volume is defined by a volume/altitude table. Each point in the table gives an altitude and the cumulative volume available to hydrodynamic materials in the CVH package below that altitude in that control volume. The volume at the lowest altitude (the bottom of the control volume) must be zero; the difference in altitude between the last point and the first one defines the height of the control volume, and the last volume entry defines its total volume. Volume is assumed to be a linear function of altitude between the table entries (see Figure 1.1). There may be an arbitrary number of entries in the table.

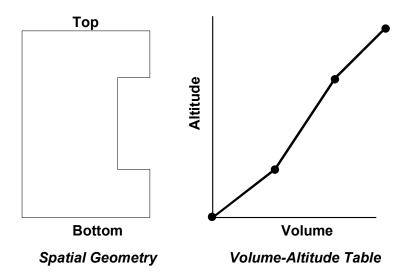


Figure 1.1 Spatial Geometry (left) and Volume/Altitude Table (right)

All altitudes input to MELCOR must be relative to a single, common, reference point to allow determination of the difference in elevations of control volumes and of the location of connections to flow paths. The same reference point must be used in the CVH, FL, Core (COR), and Heat Structure (HS) packages. Any consistent reference point may be used; consequently, both positive and negative values of altitude are allowed.

CVH input defines the volume *initially* available to hydrodynamic materials; it should *not* include either the volume occupied by intact core components or that occupied by ice in an ice condenser. Such volume is referred to as *virtual volume*, and represents space occupied by material in another MELCOR package (and therefore denied to hydrodynamic materials) that is subject to relocation. For example, when the core melts down and relocates to the lower plenum, some or all of the volume that it initially occupied will be freed, but the resulting debris will occupy space in the lower plenum. In addition to the core, core debris, and ice, water films on surfaces occupy virtual volume.

Initial values of virtual volume are defined by the package (COR or HS) that models the associated material. An initial virtual-volume/altitude table is constructed using the set of altitudes defined by CVH input, and added to the table defined by CVH input to define a *total* volume/altitude table that does not change during a MELCOR calculation. However, the virtual-volume/altitude table changes as nonhydrodynamic material is relocated, and the volume available for the hydrodynamic material, defined as the difference between total and virtual volume, changes as a function of time. This is illustrated in Figure 1.2, where core debris has been moved into the volume of Figure 1.1. Note that the tables are always based on the altitudes defined in CVH.

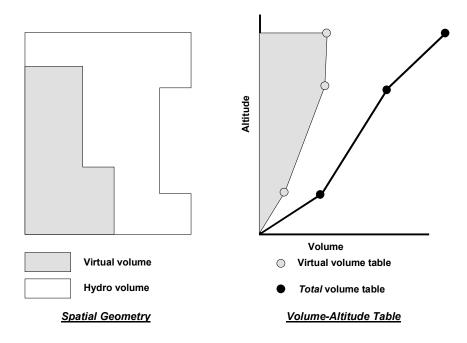


Figure 1.2 Total, Hydrodynamic, and Virtual Volume

1.2 Control Volume Contents

The contents of each control volume are divided between a so-called *pool* and an *atmosphere*, as shown in Figure 1.3. The pool is depicted as filling the lower portion of the control volume and the atmosphere filling the remainder. As discussed in the Thermal

Hydraulic (CVH and FL) Packages Reference Manual, this picture is not interpreted so narrowly that it invalidates use of MELCOR hydrodynamics in other situations.

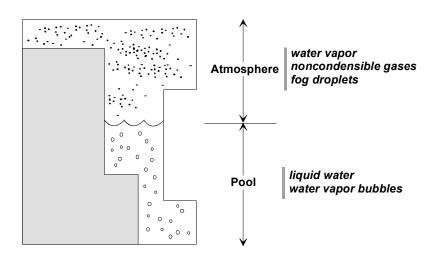


Figure 1.3 Location of Material in Control Volume

The pool can be single-phase liquid water or two-phase water. The atmosphere contains water vapor and/or noncondensible gases. The atmosphere may also have suspended water droplets (referred to as fog). Although the interactions of rising gases with the pool may be modeled (see SPARC input in the FL Users' Guide), current modeling does not permit noncondensible gases to reside in the pool. The total volume is divided among the pool, the gaseous atmosphere, and the fog.

Materials are numbered within MELCOR. Materials 1, 2, and 3 are always the pool, the fog, and water vapor in the atmosphere, respectively. Materials with numbers greater than three (if included) are noncondensible gases, and must be defined by input to the NonCondensible Gas (NCG) package.

The user can define the thermodynamic state of the material in the control volume in one of three ways:

- (1) Specify sufficient properties of the pool and the atmosphere to uniquely define—but not *over*-define—their thermodynamic states.
- (2) Define the mass and total internal energy of each material. The internal energy must be consistent with the equations of state used in MELCOR.
- (3) Specify the control volume pressure and the partial pressure of the water vapor in the atmosphere, the pool and atmosphere temperatures, water distribution in terms of mass fractions, and the mass fractions of noncondensible gases.

The first of these is the default, and will be used in most cases. The second option may be useful in defining the input to one MELCOR calculation from the output of another. The third is retained for consistency with older versions of MELCOR. Because it provides no unique capabilities and its use will often require extensive hand calculations, reference to steam tables, and/or trial-and-error iteration in MELGEN, it is not recommended for new calculations. In all cases, the input is checked for completeness and consistency. A number of details are available to reduce the amount of information which must be supplied to define, for example, a saturated volume.

1.3 Pool/Atmosphere Mass and Energy Transfer

CVH input allows two choices for thermodynamic modeling in each control volume, referred to as *equilibrium* and *nonequilibrium*; the user should be aware that the latter is *not* the same as "nonequilibrium" models in codes such as TRAC and RELAP5. Details may be found in the Control Volume Thermodynamics (CVT) Package Reference Manual. We recommend that the nonequilibrium option be used in general; the equilibrium option is retained primarily for historical reasons, but may be appropriate in special cases.

When nonequilibrium thermodynamics is used in control volume, mass and energy transfers between the pool and atmosphere are determined by the thermomechanical state of the materials in the control volume. In particular, these transfers depend on the temperatures of the pool and atmosphere, the materials in the atmosphere, the velocity of the materials, etc. The control volume hydrodynamics package calculates this energy and mass transfer between the pool and atmosphere explicitly. The transfer is decomposed into a conduction/convection mode and a boiling/flashing mode.

When equilibrium thermodynamics is specified, the transfer of mass and energy between the pool and the atmosphere is implicitly determined by the assumption that the pool and the atmosphere have equal temperatures. Thus, for example, if energy is deposited only in the atmosphere, the pool temperature will also rise and water vapor may be generated. Mass and energy transfers between pool and atmosphere are effectively instantaneous.

1.3.1 Conduction/Convection Driven Transfer

Description of phenomena at the pool surface requires simultaneous solution of the equations of heat and mass transfer. This involves finding the temperature of the pool surface which satisfies the requirements that

(1) The evaporation or condensation mass flux is that given by the mass diffusion equation for the existing gradient in the partial pressure of water vapor between the surface and the bulk atmosphere,

- (2) The net heat delivered to the interface by convection, conduction, and radiation is consistent with the latent heat required by the evaporation or condensation mass flux, and
- (3) The partial pressure of water vapor at the pool surface corresponds to saturation at the surface temperature.

The heat flows from the atmosphere to the pool surface and from the pool to the pool surface are calculated from heat transfer coefficients (subject to a lower limit defined by conduction) and the bulk pool and atmosphere temperatures. Both convection and radiation are considered in evaluating the heat transfer coefficients. Energy may also be deposited "in" the surface by other packages; this option is currently used only for radiation from the COR package. The constants in the heat transfer coefficients are defined by sensitivity coefficients in C4407(*). For more details, see the CVH/FL Reference Manual.

1.3.2 Flashing Mode Mass and Energy Transfer

A source of heat within the pool or a reduction in pressure in the control volume may result in pool boiling or flashing, respectively. Water vapor appears in the pool, steam bubbles rise to the surface, and mass and energy are transferred from the pool to the atmosphere. The remaining pool may be two phase if all the steam bubbles have not risen to the surface.

The model in the control volume package is simple. It assumes a constant bubble rise velocity, v_B , given by sensitivity coefficient C4407(1), with a default value of 0.3 m/s. It also assumes that the steam flow is a linear function of altitude in the pool, zero at the bottom, and constant throughout a timestep. These assumptions are sufficient to calculate the mass transferred to the atmosphere during a timestep. If the resulting transfer of water vapor is not sufficient to reduce the void fraction in the pool to 0.40 or below, an additional mass of water vapor is instantaneously transferred to do so. The maximum permitted void fraction is coded as a sensitivity coefficient, C4407(11). For more details, see the CVH/FL Reference Manual.

1.4 Mass and Energy Sources and Sinks

CVH input allows the definition of explicit sources and sinks (negative sources) of mass and/or energy. Additional sources and sinks may be imposed by other packages during a MELCOR calculation; these are treated automatically and do not require input to CVH. Heat sources are included from the Core (COR), Cavity (CAV), Fan Cooler (FCL), Fuel Dispersal Interactions (FDI), RadioNuclide (RN), Spray (SPR), and Heat Structure (HS) packages. Because a thermochemical reference point is used in thermodynamics, gas combustion modeled in the Burn (BUR) package does *not* involve an explicit heat source; the heat of combustion is implicit in the enthalpy functions as discussed in the CVH/FL

Reference Manual. Mass sources arise from CAV and SPR, from oxidation reactions in BUR, COR, and FDI, and from condensation/evaporation, structural degassing, and melting of ice (in ice condensers) in HS.

Explicit CVH sources may be defined in terms of data from the Control Function (CF), Tabular Function (TF), and/or External Data File (EDF) packages; multiple sources may be defined in each control volume. Each mass source is associated with a specific numbered material. An energy source is associated with either the pool or the atmosphere. The association may be either direct or implicitly defined by the appropriate phase for a coupled mass source.

Sources may be defined as integrals or as rates. Rates may be either absolute or normalized per unit mass or per unit volume. For a source that changes rapidly, the user should give serious consideration to use of the integral source (IESFLG = 0 or 1 on the CVHnnnCk input record). With these sources, the mass or energy added during each CVH advancement is defined by differences in the running integral. The total added through any point in time is therefore forced to match the desired total given by the defining tabular or control function. If rates are specified, on the other hand, an interpolated value is imposed as a constant over a CVH advancement; the integral of the interpolated values may be very different from the integral of the original data.

Energy sources and sinks may be defined independent of any mass sources, but if a mass source is present in a control volume, the associated enthalpy must be included in the energy source(s) for the corresponding phase—pool or atmosphere—of that volume. (Enthalpy must be used rather than internal energy, to account for volume work done in the addition process.) Energy sources may be combined if desired; there is no need to define an energy source for each mass source. Input checking is restricted to confirming that each volume containing a mass source contains at least one energy source.

In order to deposit mass with the enthalpy corresponding to a known temperature, the contribution to the energy source must be consistent with the corresponding equation of state in MELCOR. Reference points in MELCOR are defined so that all chemical heats of reaction are implicit in the enthalpy functions, as in JANAF tables. However, in order to allow use of the familiar Keenan and Keyes equation of state for water, the reference points for water, oxygen, and all other oxygen-containing species were modified from the JANAF values. See the H2O/NCG Reference Manual for more details.

As a result, while the user can obtain correct values for water from Keenan and Keyes steam tables, enthalpies for noncondensible gases must be calculated from data in the H2O/NCG Reference Manual. However, noncondensible gases in MELCOR are modeled as ideal gases, and the enthalpy of an ideal gas is a function of temperature only. Therefore, additional input options, IESFLG = 8 and 9 on the CVHnnnCk record, are provided to allow the user to associate a temperature with a mass source. For these options (only) the tabular or control functions which define sources are associated in pairs, with the second function of each pair defining the *temperature* of the material added by the

immediately-preceding mass source function. This is sufficient to uniquely determine the enthalpy of a noncondensible gas (but not that of water). Therefore, these options are strongly recommended for use with sources of noncondensible gases.

The temperature options are much less useful for water sources, and should be used with care (if at all). Alternate methods of source definition are recommended; an example, using a time-specified volume (see Section 1.5) is given in Section 5.

If a temperature option *is* used for water, the definition of enthalpy is made unique by making a further assumption about the state of the added water. *It is because this assumption may not correspond to the user's intentions that the temperature option is not recommended for water.* If liquid water is added (as pool, material 1, or as fog, material 2), at a temperature below the critical temperature, it is assumed to be saturated at the designated temperature. If the intention was to add subcooled water, the difference can be substantial, particularly for low temperatures and high pressures. For temperatures above critical, the enthalpy of "liquid" water will be calculated at critical density; the results will almost certainly not be what the user desired. For addition of water vapor, material 3, the enthalpy will be calculated at the designated temperature and a density corresponding to saturation at 0.1 MPa. Because water vapor is far from ideal, the result may differ significantly from that desired.

1.5 Boundary Volumes

MELCOR hydrodynamics allows thermal-hydraulic boundary conditions to be defined by specifying the state of one or more volumes as functions of time. A *time-independent* volume may be defined by simply setting a flag on record CVHnnn01 and defining its state in the same manner as for a normal volume, using CVHnnnAk records. An alternate value of this switch allows the user to define a *time-specified* volume, with properties that change as a function of time to follow a history defined by tabular functions, control functions, and/or external data files. In this case, the numeric fields on CVHnnnAk records are simply replaced by references to appropriate tabular or control functions, or data channel of an external data file.

Initialization of a calculation to the normal operating conditions in a power plant (or other facility) can be tedious because of the numerous mass, momentum, and energy balances involved. Time-independent volumes can be used to establish fixed boundary conditions; for example, the state of the pressurizer serves to define the system pressure, while that of the steam generator secondaries is critical in defining the system temperature. Other parameters will stabilize after relatively short calculations with these volumes defined as time-independent, and the results reentered as initial conditions for the transient calculation of interest.

An option is available in MELCOR 1.8.4, to define a volume as time-independent until a user-specified time is reached, at which time it is *activated* and treated thereafter as a

normal volume. This allows the initialization calculation to be performed as part of the transient calculation, with the time to end initialization defined on the optional CVHTENDINI record.

The essential difference from a normal volume is that the new state in a time-independent or time-specified volume is *defined* in the solution of the hydrodynamic equations. Any mass and/or energy sources (in addition to masses and energies advected by CVH or transferred by other packages) required to achieve that state are computed and recorded as additional sources created in the CVH package.

These volumes may be used in any way that a normal volume may be used, including definition of conditions for vapor and aerosol phenomena in the RN package. Fission products in the RN package are transported with material flows into and out of normal control volumes. They are treated as infinitely dilute in time-independent and time-specified volumes, and are therefore transported *into*, *but not out of* them. This is necessary to prevent fission products from being drawn back into a failed containment from the environment (modeled as a time-independent volume) if containment pressure falls below atmospheric pressure.

A time-specified volume may also be used to define the enthalpy of mass sources, and is particularly useful for water sources. See Section 1.4 and the example in Section 5.

2. User Input

CVH input to MELGEN defines the initial state of control volumes. There is no provision to modify conditions on restart; CVH input to MELCOR is limited to activation of additional optional output, which may be useful in identifying the source of calculational difficulties.

Several input options are included with the comment "do not use." These correspond to situations where the input will be accepted by MELCOR 1.8.4 but, because only partial coding has been provided, the option does not function properly. The information is provided as a warning to the user, because inadvertent activation of such an option could lead to a code failure that might be difficult to diagnose.

2.1 MELGEN User Input

The user input for the control volume hydrodynamics package is described below. The first set of input (CVTYPEnn records) is optional and is used to defined general types of control volumes for editing and accounting purposes (currently only used in the RN package edit routine). The second set of input (CVnnnXX records) is required and is used to describe each individual control volume defined for the given application. Up to 999 control volumes may be defined. Practically, the number is limited only by the available memory on the computer. Unless otherwise stated, if the field variable starts with I through N, it is an

integer. Unless otherwise stated, if the field variable starts with A through H or O through Z, it is a real number.

CVHTENDINI – Time to end initialization Optional

The ICVACT input on record CVHnnn01 may be used to declare volumes as time-independent for an initialization segment of a calculation to allow stabilization of normal operating conditions in a power plant or other facility. With ICVACT = -3, this record defines the end of the initialization period; if absent, any volume so declared will be activated at the start of the MELCOR calculation. See discussion in Section 1.5.

(1) TENDIN - Time to end initialization and activate all volumes with ICVACT = -3 (type = real, default = TSTART, units = s)

CVTYPEnn – Control volume type names

 $01 \le nn \le 99$, nn is the control volume type number (ICVTYP) associated with input records CVnnn00 described below and with the control volume type number (ICVTYP) on RN input record RN2FLTxx00 Optional

This record allows the user to associate customized names with groups of related CVH package control volumes or RN package filters. For example, each of the control volumes associated with the reactor coolant system might be assigned ICVTYP=3 on the CVnnn00 record (described below) for each control volume in the group, and then this record would appear here as: CVTYPE03 'RCS.'

(1) CVTYPE - User defined control volume type name. (type = character*7, default = TYPEnn for nn < 99, or default = FILTERS for nn = 99)

CVnnn00 – Control volume name and switches

 $1 \le nnn \le 999$, nnn is the user-assigned control volume number Required

This record defines the name of the control volume and the attributes of the control volume.

(1) CVNAME - User defined control volume name. (type = character*16, default = none)

- (2) ICVTHR Control volume thermodynamics switch. The nonequilibrium option is recommended in general.
 - = 1 equilibrium (Tpool = Tatmos)
 - = 2 nonequilibrium (Tpool ≠ Tatmos)

(type = integer, default = none, units = dimensionless)

- (3) ICVFF
- Control volume flow flag. This flag is currently unused, but an input value from the following list must be specified.
 - = 0 not defined
 - = 1 horizontal flow
 - = 2 vertical flow

(type = integer, default = none, units = dimensionless)

- (4) ICVTYP
- Type of control volume. This entry must be an integer between 1 and 99, inclusive. It is used to defined groups of associated control volumes for editing and accounting purposes only (currently only the RN package editing/accounting routine uses this flag to permit editing by CV type; see the RN Users' Guide for more information). The user may define a name to be associated with each type of control volume specified by this entry by including the CVTYPEnn records described above. By default the name associated with control type nn is TYPEnn for 01 ≤ nn ≤ 98, while control type 99 is reserved for FILTERS by default. (type = integer, default = none, units = dimensionless)

CVnnn01 – Control volume switches

 $1 \le nnn \le 999$, nnn is the user-assigned control volume number Optional

This record allows the user to specify that no fog may exist in the control volume atmosphere. In this case, all water will be put into the pool.

A volume may also be declared "time-independent" or "time-specified." A volume may further be declared to be "time-independent" only during an initialization segment of a calculation, and become a normal volume thereafter. See discussion in Section 1.5. The time to end initialization is defined on the CVHTENDINI record.

Other options, marked "do not use" are listed. While the input may be accepted by the input processor, the models are incomplete, and do not function correctly.

- (1) IPFSW
- Pool/no pool, fog/no fog switch.
 - = 0 pool, fog allowed (default)
 - = 1 no pool, fog allowed** do not use**
 - = 2 pool allowed, no fog (any liquid water is moved to pool)\

(type = integer, default = none, units = dimensionless)

- (2) ICVACT Active/inactive switch.
 - = 0 active, with state advanced by integrating the conversation equations, (default)
 - = 1 inactive** do not use**
 - = -1 time-independent
 - = -2 properties specified as a function of time
 - = -3 equivalent to -1 (time-independent) for TIME < TENDIN, and to 0 (active) for TIME ≥ TENDIN. TENDIN is defined on record CVHTENDINI

(type = integer, default = 0, units = dimensionless)

CVnnn02 – Control volume initial velocities

 $1 \le nnn \le 999$, nnn is the user-assigned control volume number Optional

Average velocities in the control volume atmosphere and pool are used by the CVH, COR, and HS packages in calculation of heat transfer coefficients. This record may be used to define nonzero initial values of these velocities, which will be used until internally calculated values become available during the first advancement in MELCOR.

- (1) VLATMO Velocity of atmosphere. (type = real, default = 0.0, units = m/s)
- (2) VLPOLO Velocity of pool. (type = real, default = 0.0, units = m/s)

CVnnn03 – Control volume area for velocity calculation

 $1 \le nnn \le 999$, nnn is the user-assigned control volume number Optional

During advancement, the velocities in each control volume are internally calculated from the area of the control volume and the area, void fraction and velocities in the flow paths connected to that control volume. The default value for the control volume area is given by its volume divided by its height.

(1) CVARA - Control volume area used for velocity calculation. (type = real, default = volume/height, units = m²)

CvnnnA0 – Switch for type of thermodynamic input

 $1 \leq nnn \leq 999, \, nnn$ is the user-assigned control volume number Optional

The user must provide sufficient information to define the initial thermodynamic state of the control volume. The fundamental internal variables in MELCOR are mass and internal energy, but options are provided which allow the user to specify the state in terms of more commonly available quantities. If these options are employed, the user-input quantities are used to calculate mass and energy. These are then used as arguments to the equation of state in the Control Volume Thermodynamics package, which may not reproduce input pressures and temperatures exactly. In addition, if nonequilibirum conditions (unequal pool and atmosphere temperatures) are input for a volume in which equilibrium thermodynamics is specified (ICVTHR = 1 on record CVnnn00), the input will be processed and the resulting (nonequilibrium) contents equilibrated. Three input options are available:

- (1) Direct mass and energy input. This option is useful primarily for matching conditions in previously-performed MELCOR calculations.
 - Input the mass and total internal energy of each material present. The internal energy must be consistent with equations of state used in MELCOR with respect to the thermochemical reference point employed.
- (2) Pressures, temperatures, and mass fractions input. This option is retained for compatibility with MELCOR versions prior to 1.7.0.
 - Input pressures and/or temperatures. Specify the location of water as mass fractions in the pool, fog, and/or atmosphere. Specify the composition of the noncondensible gas in the atmosphere as mass fractions. Actual amounts of all materials are then inferred from pressures and temperatures.
- (3) Separate pool and atmosphere input. This option is recommended for normal applications. <u>It is the only option permitted for time-specified volumes (ICVACT = -2 on the CVnnn01 record).</u>

Input pressures and/or temperatures. Specify the amount of pool as a mass, volume, or surface elevation. Specify the composition of the atmosphere in terms of its water content (partial pressure, relative humidity, or dewpoint temperature) and the mole fractions of noncondensible gases. An initial void fraction in the pool and/or fog content in the atmosphere may also be specified.

- (1) ITYPTH Type of thermodynamic input (type = integer, default = 3, units = dimensionless)
 - = 1 material masses and energies
 - = 2 pressures, temperatures, and mass fractions
 - = 3 separate pool and atmosphere input

CVnnnAk – Thermodynamic input

 $1 \le nnn \le 999$, nnn is the user-assigned control volume number

 $1 \le k \le Z$, k is a sequencing character

Required

The thermodynamic input consists of data pairs. The first datum is a character variable identifying the quantity input, and the second is a real number giving its value. The character variable (first datum) may be constructed from one or two fields; if two, the second is a material number, separated from the first by a period. Both elements of a data pair must be on the same record.

Recall that

n = 1 is pool.

n = 2 is fog (liquid water in atmosphere).

n = 3 is water vapor in atmosphere.

n = 4,5,... are noncondensible gases (identified by input to the NCG package), and that MELCOR pressures are defined at the pool/atmosphere interface, the top of the pool or bottom of the atmosphere.

The input variables required, and the treatment of defaults, are different for each type of thermodynamic input (ITYPTH). The input for time-independent volumes is the same as for normal volumes; that for time-specified volumes is discussed following the description of input for ITYPTH = 3.

For ITYPTH = 1 (Mass and energy input)

ETOT.n - Total internal energy of material n. (type = real, default = 0.0, units = J)

MASS.n - Mass of material n. (type = real, default = 0.0, units = kg)

For ITYPTH = 2 (Mass fraction input)

Input the total volume pressure, the partial pressure of water vapor in the atmosphere, and the temperatures of the pool and of the atmosphere. Specify the partition of water among pool, atmosphere, and fog as water mass fractions; the actual masses are implicitly defined by the temperatures, the pressures and the total volume. (If both water vapor and fog are present, the partial pressure of water in the atmosphere must correspond to saturation at the atmosphere temperature.)

Specify the composition of the noncondensible gas in the atmosphere as noncondensible gas mass fractions; the actual amounts are implicitly defined by the difference between the partial pressure of water vapor in the atmosphere and the total pressure. The control volume pressure is defined as the pressure at the

pool/atmosphere interface. If not pool is present, it is the pressure at the lowest elevation in the cell. If no atmosphere is present, it is the pressure at the highest elevation of the cell.

MFRC.n

- Mass fraction of material n. If water is present, the mass fractions for materials 1 through 3 must sum to 1.0. If noncondensible gases are present, the mass fractions for materials 4,... must sum to 1.0.

(type = real, default = 0.0, units = dimensionless)

PVOL

Control volume pressure (pool pressure if a pool is present). Must be input if a pool is present (MFRC.1 > 0.0). If there is no pool, and PVOL is not input, the pressure in the control volume will be set to the pressure of water vapor in the atmosphere. In this case, no noncondensible gas is allowed.
 (type = real, default = see discussion, units = Pa)

PH2O

- Partial pressure of water vapor in the atmosphere. If negative, the partial pressure of water vapor will be set to the input total volume pressure (PVOL); if PVOL is not input (permitted if there is no pool), PH2O is interpreted as the total pressure. In either case, no noncondensible gases are allowed. PH2O should be input as 0.0 if there is no pool and no water is present in the atmosphere. (type = real, default = see discussion, units = Pa)

TATM

Temperature of atmosphere. If negative or not input, the saturation temperature at the partial pressure of water in the atmosphere (PH2O) will be used.
 (type = real, default = -1.0, units = K)

TPOL

 Temperature of pool. If negative or not input, the temperature of the pool is set to saturation at the pool pressure (PVOL). (type = real, default = -1.0, units = K)

For ITYPTH = 3 (Separate pool and atmosphere input)

Pool Input

If a pool is present, specify the amount of pool using one (and only one) of the following (if there is no pool, *none* of these variables should be input):

MASS.1 - Mass of pool. (type = real, default = 0.0, units = kg)

VPOL - Volume of the pool. (type = real, default = 0.0, units = m³) ZPOL - Elevation of the pool surface. (type = real, default = none, units = m)

If a pool is present, specify its thermodynamic state: specify both its pressure *and* temperature (less than saturation for the given pressure) if subcooled; either its pressure *or* temperature if saturated. If it is subcooled, the pressure may be defined by the corresponding saturation temperature. If it is saturated, an initial void fraction may also be defined.

PVOL

Control volume (pool) pressure. If zero, negative, or not input, the volume pressure is set to saturation at either TSAP, if input, or at the pool temperature (TPOL).
 (type = real, default = 1.0, units = Pa)

TPOL

Temperature of pool. If zero, negative, or not input, the temperature of the pool is set to saturation at the pool pressure (PVOL).
 (type = real, default = -1.0, units = K)

TSAP

Saturation temperature of pool, used to define the pressure (which is also the total control volume pressure). If both PVOL and TSAP are zero, negative, or not input, the pressure of the pool is set to saturation at the pool temperature (TPOL).
 (type = real, default = -1.0, units = K)

VOID

Void fraction in the pool, in the range 0.0 ≤ VOID < 1.0. Because noncondensibles may not reside in the pool, any bubbles must be water vapor. Therefore, input of VOID is permitted only for a saturated pool. If not input, the pool void fraction will be zero. (type = real, default = 0.0, units = dimensionless)

The atmosphere, including fog if present, then occupies the remainder of the control volume. *If the pool fills the volume (as specified by VPOL or ZPOL), no atmosphere properties may be input.* If a pool is present, the volume pressure has already been defined; if *no* pool is present, the control volume pressure must still be specified.

PVOL

Control volume pressure. If zero, negative, or not input, and not defined by pool input (as saturation at the pool temperature), the volume pressure is set to saturation at the atmosphere temperature (TATM), which must then be included in the input. (type = real, default = -1.0, units = Pa)

Atmosphere Input

If an atmosphere is present: specify both the partial pressure of water vapor in the atmosphere (directly or by the relative humidity or the dewpoint temperature) and the temperature (greater than saturation for the given vapor pressure) if the atmosphere is superheated; specify only the partial pressure of water or the temperature if it is saturated. Note that input of a non-negative value for PH2O or of a value for either RHUM or TDEW fully defines the water vapor content of the atmosphere. Over-specification (by input of more than one of these) is not permitted.

PH2O

 Partial pressure of water vapor in the atmosphere. If negative or not input, the partial pressure of water in the atmosphere will be set to saturation or to an optionally input relative humidity (RHUM) at the atmosphere temperature (TATM), or to saturation at an optionally input dewpoint temperature (TDEW), one of which must then be input.

(type = real, default = -1.0, units = Pa)

RHUM

Relative humidity of the atmosphere, in the range 0.0 ≤ RHUM ≤ 1.0. Relative humidity is defined as the ratio of the partial pressure of water vapor to saturation pressure at the atmosphere temperature.

(type = real, default = 1.0, units = dimensionless)

TATM

Temperature of atmosphere. If zero, negative, or not input, the saturation temperature at the partial pressure of water in the atmosphere (PH2O) will be used.
 (type = real, default = -1.0, units = K)

TDEW

 Dewpoint temperature in the atmosphere. The dewpoint temperature is defined as the saturation temperature corresponding to the partial pressure of water vapor. (type = real, default = none, units = K)

If noncondensible gas is present in the atmosphere, specify its composition as mole fractions; the actual amounts of the various gases are implicitly defined by the difference between the partial pressure of water vapor in the atmosphere and the total pressure. If this difference is zero, no input is permitted.

MLFR.n

Mole fraction of noncondensible gas n. Used only for ITYPTH =
 3. If noncondensible gases are present (not present), the sum for materials 4,... should equal 1.0 (0.0).
 (type = real, default = 0.0, units = dimensionless)

If an atmosphere is present, and the partial pressure of water vapor corresponds to saturation for its temperature, optionally specify the fog content either directly by its mass or indirectly by the volume fraction in the total atmosphere (but not both).

MASS.2 - Mass of fog. (type = real, default = 0.0, units = kg)

VFOG - Volume fraction of fog in the atmosphere in the range 0.0 ≤ VFOG < 1.0.
 (type = real, default = 0.0, units = dimensionless)

For Time-Specified Volumes

The properties of a volume may be specified as user-defined functions of time by setting ICVACT = -2 on record CVnnn01. The permitted input variables are a subset of those described above for ITYPTH = 3 (which is the only permitted value of ITYPTH for this type of volume). The same keywords (PVOL, etc.) are used, but with a function or file reference replacing the constant value. Permitted references are TF.n, CF.n, or EDF.n.m, denoting tabular function n, control function n, or channel m of external data file n, respectively. A constant value must be specified by reference to a constant tabular or control function or a constant EDF data channel.

Keywords that are currently recognized are PVOL, ZPOL, TPOL, VOID, TATM, PH2O, and MLFR.n. They are interpreted as follows:

PVOL - Control volume pressure. Required. (type = real, default = none, unit = Pa)

ZPOL - Elevation of pool surface. Optional. If absent, no pool will ever be present, and input of TPOL or ZPOL is not permitted. (type = real, default = none, unit = m)

TPOL

- Temperature of pool. Optional, permitted only if ZPOL is input. Note that TPOL must be specified if a subcooled pool will ever be present. During periods when there is no pool (as specified by ZPOL), the value of TPOL will not be used. When a pool is present, a value of TPOL equal to or not more than C4409(6) (default, 1.0 K) above saturation of PVOL will be interpreted as saturation. Any greater superheat will result in termination of the calculation. Note that MELCOR thermodynamics does not permit a superheated pool; the tolerance on input is intended only to accommodate minor discrepancies resulting from interpolation in tabular data when a saturated pool is intended.

If ZPOL is input and TPOL is not, the pool (if present) will be saturated at PVOL.

(type = real, default = -1.0, unit = K)

VOID

Void fraction in the pool. Optional, permitted only if ZPOL is input. Ignored unless the pool is saturated. If not input, the pool void fraction will be zero.
 (type = real, default = 0.0, unit = dimensionless)

TATM

- Temperature of atmosphere. Optional. If an atmosphere is present and TATM is not input, the atmosphere will consist of saturated water vapor at PVOL. Note that TATM must be specified if the atmosphere will ever be superheated or contain noncondensible gases. It is impossible for input checking to assure that PVOL and TATM will always specify a superheated state. Therefore, if TATM is specified, the composition of noncondensibles (MLFR.n) must also be specified, see below. (type = real, default = 1.0, unit = K)

PH2O

- Partial pressure of water vapor in the atmosphere. Optional, currently permitted only if TATM is input. In execution, a value of PH2O corresponding to saturation at TATM or at a temperature not more than C4409(6) (default, 1.0 K) below TATM will be interpreted as saturation at TATM. Any greater subcooling will result in termination of the calculation. Note that MELCOR thermodynamics does not permit a supersaturated atmosphere; as discussed for keyword TPOL, the tolerance on input is intended only to allow for imprecision in interpolation. If TATM is input and PH2O is not, the partial pressure will be the minimum of PVOL and saturation at TATM.

(type = real, default = 1.0, unit = Pa)

MLFR.n

Mole fraction of noncondensible gas n (n ≥ 4). Required if TATM is input, not permitted otherwise. (If TATM is input, <u>both</u> P and T will be specified. If input, the values must sum to 1.0 within C4409(5) (default, .001); the tolerance allows for some imprecision in interpolation of tabular data.

(type = real, default = 0.0, unit = dimensionless)

The tabular function, control function, or external data file should define the variable as a function of time in the appropriate SI units. For example, given the input

PVOL EDF.101.3

channel 3 of external data file 101 should contain the desired pressure in Pascals.

CVnnnBk – Altitude/volume table

 $1 \leq nnn \leq 999,$ nnn is the user-assigned control volume number $0 \leq k \leq Z,$ k is a sequencing character Required

The input data are altitude-hydrodynamic volume pairs. The first element of a pair is the altitude and the second is the volume initially available to be occupied by material in the CVH package (free volume). Virtual volume is not included in these input data. At least two pairs (four numbers) must be input. The volume corresponding to the lowest elevation must be zero. For other data pairs: if the input volume is positive, it is interpreted as the total volume between the bottom (lowest elevation input) and the current input elevation; if it is negative, the absolute value of the volume is interpreted as the volume change from the next-lower input elevation.

Multiple data pairs may be on one record, limited only by the permitted length of input records (100 characters). A data pair may not be split between two records. (type = real, default = none, units = m and m^3)

CVnnnCk – External Mass and Energy Sources

 $1 \leq nnn \leq 999,$ nnn is the user-assigned control volume number $0 \leq k \leq Z,$ is a sequencing character Optional

These records are used to define user input mass and energy (enthalpy) sources and sinks, in addition to those calculated by other packages. As discussed in Section 1.4, such sources may be prescribed using control functions, tabular functions or external data files. Two formats are allowed; the first (original) format permits only control or tabular functions. The second allows additional options, including use of external data files and imposition of a scaling factor, but does not allow use of a temperature to specify the energy associated with a mass source.

Format 1

Each record consists of an identifier field, a character field specifying the destination of the mass or energy, the tabular function or control function number and a switch specifying the interpretation of the function.

Mass and energy sources may, in general, be defined independently so long as the enthalpy associated with each mass source is properly accounted for. However, a "TE" type source defines an energy source in terms of the temperature of an associated "MASS.n" source. This mass source must immediately precede the "TE" source when the list of sources for the control volume is ordered according to record

identifiers (that is, by the sequencing character k in CVnnnCk). If this requirement is not met, and there is no "MASS.n" source record immediately preceding a "TE" source record, MELGEN will trap the error, write a diagnostic, and not write a cycle zero restart.

The only values of the input switch IESFLG that may be used with a "TE" source are 8 and 9; conversely, these values may only be used with a "TE" source. These sources are *not* recommended for use with water. See the discussion in Section 1.4.

- (1) CTYP Character field defining mass or energy source.
 - AE External enthalpy source for the atmosphere.
 - PE External enthalpy source for the pool
 - TE Specific enthalpy of the previous mass source is defined as a function of temperature. Temperature is defined by the tabular function or control function. An atmosphere or pool destination is determined by the mass source.
 - MASS.n Mass source for material n (as always, material 1 is pool, 2 is fog, 3 is atmospheric vapor, and $n \ge 4$ is a noncondensible gas identified by input to the NCG package).

(type = character*8, default = none)

- (2) IESTYP The control function or tabular function numbers associated with the third field (IESFLG).
 (type = integer, default = none, units = dimensionless)
- (3) IESFLG Input switch.
 - = 0 Use tabular function IESTYP for cumulative source through the current time.
 - = 1 Use control function IESTYP for cumulative source through the current time.
 - = 2 Use tabular function IESTYP for source rate.
 - = 3 Use control function IESTYP for source rate.
 - = 4 Use tabular function IESTYP for source rate per unit mass.
 - = 5 Use control function IESTYP for source rate per unit mass.
 - = 6 Use tabular function IESTYP for source rate per unit volume.
 - = 7 Use control function IESTYP for source rate per unit volume.
 - = 8 Use tabular function IESTYP for temperature to define specific enthalpy of immediately-preceding mass source.

 Use control function IESTYP for temperature to define specific enthalpy of immediately-preceding mass source.
 (type = integer, default = none, units = dimensionless)

Format 2

Each record consists of an identifier field, a character field specifying the type of source, a field specifying whether the data are rates or integrals, a field specifying the source of the data, and an optional scale factor for that data.

(1) CTYP - Type of source.

ENERGY.A Enthalpy source for the atmosphere.

ENERGY.P Enthalpy source for the pool.

MASS.n Mass source for material n (as always, material

1 is pool, 2 is fog, 3 is atmospheric vapor, and n \geq 4 is a noncondensible gas identified by input

to the NCG package).

FILE Vector of mass and enthalpy sources, obtained

from an external data file. The optional FLnnn06 record can be used to record the mass and enthalpy flows through a flow path in an appropriate format for this use, with the

INTEGRAL option below.

(type = character*8, default = none)

(2) INTERP - Interpretation of source data.

RATE Data are to be interpreted as rates (W or kg/s)
INTEGRAL Data are to be interpreted as cumulative (J or kg)

(type = character*8, default = none)

(3) IESSRC - Character field defining location of source data.

For ENERGY.f or MASS.n sources:

CF.nnn Data from control function nnn
TF.nnn Data from tabular function nnn

EDF.nnn.iii Data from channel iii of external data file nnn

(type = character*11, default = none)

For FILE sources:

EDF.nnn Data from external data file nnn, which must

contain at least NUMMAT+2 channels (where NUMMAT is the number of materials in the problem). Of these, the first NUMMAT+2 channels will be used as data for MASS.1, MASS.2, ..., MASS.NUMMAT, ENERGY.P and

ENERGY.A sources, in that order.

(4) ESSCAL - Scale factor for data from IESSRC. (type = real, default = 1.0, units = dimensionless)

2.2 MELCOR User Input

The CVH database cannot be modified at a MELCOR restart at this time. However, a diagnostic tracing option may be activated as an aid in identifying problem areas in a calculation.

CVHTRACE – Calculational trace activation Optional

If this record is present, the progress of the solution of the CVH hydrodynamic equations will be tracked, and informative messages will be written to the diagnostic file (MELDIA). See Section 7.2 for a discussion of these messages. The output is voluminous, and the trace should only be activated for short runs. Presence of the CVHTRACE record is *not* recorded in the restart file. Therefore, the trace is active if and only if this record is present in MELCOR input for the current execution.

3. Sensitivity Coefficients

The *sensitivity coefficient* feature in MELCOR is a powerful feature that gives the user the ability to change selected parameters the physics models that would otherwise require modification of the Fortran source code. Their use is described in Section 7 of the MELCOR EXEC Users' Guide.

3.1 CVH Sensitivity Coefficients

The sensitivity coefficients for all hydrodynamic modeling involving the CVH and FL packages have identifier numbers from 4400 to 4599. This section contains brief descriptions of these sensitivity coefficients. Additional information, including references for models and equations, may be found in the Thermal Hydraulic (CVH and FL) Packages Reference Manual; Appendix A in that Reference Manual provides information to aid in locating the specific locations where each sensitivity coefficient is discussed.

The CVH package may use two or more smaller steps to advance through a MELCOR system timestep; each such step is referred to as *subcycle*. Timestep controls are based on changes over the system timestep. If an iteration fails to converge, or if an error is encountered in the thermodynamics, CVH will attempt to repeat the calculation with a reduced subcycle step before modifying the MELCOR system timestep.

Several sensitivity coefficients in the CVH database are currently unused. Input for unused coefficients is accepted (for compatibility with older versions of MELCOR), but has no effect on the calculation. For completeness, these coefficients are still listed in the discussion below.

4400 - Timestep Control

These coefficients are used to control the system timestep. Array elements 4-11 are used to define limits on the maximum change desired or permitted in the pressure or temperature in any volume during a single timestep. For example, the CVH package will attempt to control the maximum pressure change in any volume to satisfy $|P^n - P^o| \le C4400(4) P + C4400(5)$ by requesting a system timestep for the *next* timestep such that this condition would not be violated for the rates of change calculated on the last completed timestep. If, however, the result on completion of a timestep is that $|P^n - P^o| > C4400(6) P + C4400(7)$ for some volume, CVH will request a MELCOR fallback, and the entire advancement will be repeated with an appropriately reduced timestep. Changes in pool and atmosphere temperatures are treated similarly.

The default values for C4400(4-11) were chosen to permit a safety factor of roughly 2 between the desired maximum changes and the changes which will lead to a fallback. A similar safety factor should be maintained if the default values are modified.

- (1) Maximum fraction of material Courant timestep allowed.
 (default = 0.5, units = dimensionless, equiv = DTFRCC)
- Timestep reduction fraction used when the number of significant digits from the matrix solver is less than two. If the matrix is poorly conditioned, the number of significant digits for the velocities may be so small as to be meaningless. When the number of significant digits is less than two, then the system timestep will be reduced for the next cycle. (default = 0.9, units = dimensionless, equiv = DTFRCD)
- The fraction of the (old) system timestep used when the equation of state package returns an error for a calculation involving no flow paths; the cycle is repeated with the system timestep cut to this fraction of its previous value. (For a calculation involving flow paths, CVH will first reduce the subcycle step.)
 (default = 0.15, units = dimensionless, equiv = DTEOSF)
- Relative change contribution to the maximum desired pressure change in any volume during a single timestep. Used with C4400(5).

(default = 0.05, units = dimensionless, equiv = DPROK)

- Absolute change contribution to the maximum desired pressure change in any volume during a single timestep. Used with C4400(4).
 (default = 0.0, units = Pa, equiv = DPAOK)
- Relative change contribution to the maximum permitted pressure change in any volume during a single timestep. Used with C4400(7).
 (default = 0.1, units = dimensionless, equiv = DPRCUT)
- Absolute change contribution to the maximum permitted pressure change in any volume during a single timestep. Used with C4400(6).
 (default = 0.0, units = Pa, equiv = DPACUT)
- (8) Relative change contribution to the maximum desired temperature change in any volume during a single timestep. Used with C4400(9).
 (default = 0.1, units = dimensionless, equiv = DTROK)
- (9) Absolute change contribution to the maximum desired temperature change in any volume during a single timestep. Used with C4400(8). (default = 1.0, units = K, equiv = DTAOK)
- (10) Relative change contribution to the maximum permitted temperature change in any volume during a single timestep. Used with C4400(11).
 (default = 0.2, units = dimensionless, equiv = DTRCUT)
- (11) Absolute change contribution to the maximum permitted temperature change in any volume during a single timestep. Used with C4400(10).
 (default = 1.0, units = K, equiv = DTACUT)

4401 – Velocity Convergence Criteria

The velocities are calculated by inverting a system of linear equations. The coefficients in the matrix and the inhomogeneity vector are functions of the velocity. The velocities are iterated until the difference between successive iterates is sufficiently small that $|v'-v'^{-1}| \le C4401(1) ||v'|+|v'^{-1}|| + C4401(2)$ for all flows (the superscript refers to the iteration number). Additional tests identify reversed flows.

- (1) Relative convergence criterion.(default = .09, units = dimensionless, equiv = CVELR)
- Absolute velocity convergence criterion.
 (default = 0., units = m/s, equiv = CVELA)

- Maximum number of iterations permitted before solution is repeated with a decreased (subcycle) timestep. The default value of 0.0 is used to specify a limit scaled to the size of the problem; the actual value used is 8. + the number of flow paths in the nodalization.
 (default = 0., units = dimensionless, equiv = XPASMX)
- Number of iterations after which velocities will be considered converged if there is no significant effect (less than 0.05%) on pressures. A value of 0.0 gives the default treatment, which is not to consider the relaxed convergence criterion. (*Treatment in versions prior to 1.8.2 corresponded to a value of 8.0.*)
 (default = 0.0, units = dimensionless, equiv = XPASP)

4402 – Minimum velocity to be considered for choking calculation

Velocities calculated from the flow (momentum) equations subjected to limits imposed by critical flow correlations. The tests will be bypassed unless either the pool velocity or the atmosphere velocity is greater than a threshold value.

Velocity below which choking tests are bypassed.
 (default = 20., units = m/s, equiv = CVELMN)

4403 - Not used

4404 – Friction Factor Parameters

A two phase friction factor is calculated for each flow path segment. Laminar flow is assumed if the Reynolds number is less than C4404(14), turbulent flow is assumed if the Reynolds number is greater than C4404(15), and a transition region for Reynolds numbers between these values. The friction factor for laminar flow is determined by dividing the value of the variable SLAM by the value of the Reynolds number. The default value of SLAM is C4404(13). The Colebrook-White equation

$$\frac{1}{\sqrt{f}} = C4404(1) - C4404(2)\log_{10}\left(C4404(3)\frac{e}{D} + \frac{C4404(4)}{\text{Re}\sqrt{f}}\right)$$

is used to define the friction factor, f, for turbulent flow, where e is the surface roughness and D is the hydraulic diameter.

Re is the Reynolds number based on the hydraulic diameter and a two-phase mixture viscosity, $\mu_{\rm M}$, defined by

$$\mu_{\rm M} = \mu_{\rm P} [{\rm C4404(6)} - \alpha] [{\rm C4404(10)} + {\rm C4404(11)} \ \alpha] + \alpha \mu_{\rm A}$$

where μ_P is the pool viscosity, α is the void fraction, and μ_A is the atmosphere viscosity. Note that, if C4404(6) = 1.0, it has the proper limits for $\alpha \to 0.0$ and $\alpha \to 1.0$.

- (1) Coefficient in Colebrook-White correlation.(default = 3.48, units = dimensionless, equiv = none)
- (2) Coefficient in Colebrook-White correlation.
 (default = 4.0, units = dimensionless, equiv = none)
- (3) Coefficient in Colebrook-White correlation. (default = 2.0, units = dimensionless, equiv = none)
- (4) Coefficient in Colebrook-White correlation.
 (default = 9.35, units = dimensionless, equiv = none)
- (5) Value used in iterative solution. Should not be modified. (default = 1.0/ln(10) = 0.43429448190325182765, units = dimensionless, equiv = none)
- (6) Coefficient in two-phase viscosity correlation. Must be 1.0 to get proper limit for $\alpha = 1.0$. (default = 1.0, units = dimensionless, equiv = none)
- (7) Value used in iterative solution. <u>Should not be modified</u>.
 (default = 14.14, units = dimensionless, equiv = XINOLD)
- (8) Value used in iterative solution. <u>Should not be modified</u>. (default = 0.0005, units = dimensionless, equiv = RELC)
- (9) Value used in iterative solution. <u>Should not be modified</u>.
 (default = 0.0, units = dimensionless, equiv = RELA)
- (10) Coefficient in two-phase viscosity equation.(default = 1.0, units = dimensionless, equiv = none)
- (11) Coefficient in two-phase viscosity equation. (default = 2.5, units = dimensionless, equiv = none)

- (12) If the void fraction is less than this number, the atmosphere friction factor is set to zero. For greater void fractions, the atmosphere friction factor is linearly interpolated between zero and the value given by the basic model. (default = 0.9, units = dimensionless, equiv = none)
- (13) Default coefficient for calculating laminar flow friction factor. (default = 16.0, units = dimensionless, equiv = none)
- (14) Maximum value of Reynolds number for laminar flow. (default = 2000.0, units = dimensionless, equiv = none)
- (15) Minimum value of Reynolds number for turbulent flow. (default = 5000.0, units = dimensionless, equiv = none)

4405 – SPARC Bubble Physics Parameters

The user may specify on an FLnnn02 input record that mass and energy exchange terms should be calculated for hot gases entering a pool from a flow path which connects to a control volume below the pool surface in that volume. Such gases are not considered to reside in the pool, but their interactions will be accounted for before the exiting gases are allowed to join the atmosphere in the control volume. Parametric models are used in MELCOR; efficiency terms are calculated to account for bubble rise distance and liquid subcooling. The bubble rise efficiency is given by

$$\varepsilon_z = \max \left\{ 0.0, \min \left[1.0, \frac{\Delta z - C4405(1)}{hC4405(2)} \right] \right\}$$

where z is the distance that bubbles rise through the pool and h is the flow path opening height. The water temperature efficiency is given by

$$\varepsilon_{T} = \max \left\{ 0.0, \min \left[1.0, \frac{T_{sat}(P) - T_{P} - C4405(3)}{C4405(4)} \right] \right\}$$

where $T_{\rm sat}(P)$ is the saturation temperature at total pressure and $T_{\rm P}$ is the pool temperature. The net efficiency used is the product of $\varepsilon_{\rm z}$ and $\varepsilon_{\rm T}$.

(1) - Zero efficiency bubble rise height.(default = 0.01, units = m, equiv = DZZERO)

- Full efficiency bubble rise height in terms of flow path junction heights.
 (default = 1.0, units = dimensionless, equiv = DZEFF)
- Zero efficiency temperature difference between the pool and saturation temperatures.
 (default = 0.1, units = K, equiv = DTMPZR)
- Full efficiency temperature difference between the pool and saturation temperatures.
 (default = 5.0, units = K, equiv = DTEFF)
- (5) Relative humidity of the steam at the surface. (default = 0.99, units = dimensionless, equiv = PEFF)

4406 - Maximum Allowed Fog Density

The maximum mass of liquid water in the atmosphere (fog) divided by the volume of the atmosphere that will not be permitted to be larger than FOGDEN. Any excess liquid water is moved to the pool.

- Maximum fog density.
 (default = 0.1, units = kg/m³, equiv = FOGDEN)

4407 – Pool/Atmos Heat/Mass Transfer Parameters

Energy and mass transfer occurs between the pool and atmosphere of a nonequilibrium volume when their temperatures differ. The models used are outlined briefly in Section 1.3 of this report, and described in greater detail in the CVH/FL Reference Manual.

The heat transfer coefficient for each phase is given by

$$h = \max(h_{forced}, h_{free})$$

Here h_{forced} is given by the TRAC correlation for horizontal stratified flow,

$$h_{\textit{forced}} = C4407(2) \rho_{\varphi} c_{p,\varphi} v_{V,\varphi}$$

and h_{free} from the correlations for natural (free) convection for horizontal surfaces

$$h_{\text{free},A} = \max \left[\text{C4407(3)} \left(\text{Gr Pr} \right)^{\text{C4407(4)}}, \text{C4407(5)} \left(\text{Gr Pr} \right)^{\text{C4407(6)}} \right] \frac{k_A}{X_A}$$

$$h_{\text{free},P} = \max \left[\text{C4407(7)} \left(\text{Gr Pr} \right)^{\text{C4407(8)}}, \text{C4407(9)} \left(\text{Gr Pr} \right)^{\text{C4407(10)}} \right] \frac{k_P}{X_P}$$

where ρ is density, c_p is specific heat, v_V is volume velocity, k is thermal conductivity, X is characteristic length, φ refers to the phase (pool (P) or atmosphere (A)) and Gr and Pr are the Grashof and Pr and Pr and Pr are the Grashof and Pr and Pr are the Grashof and Pr and Pr are the Pr and Pr are the Pr and Pr are the Pr and Pr and Pr are the Pr are the Pr and Pr are the Pr are the Pr and Pr are the Pr and Pr are the Pr are the

- (1) Bubble rise velocity.(default = 0.3, units = m/s, equiv = VELBUB)
- (2) Coefficient for TRAC heat transfer coefficient correlation.
 (default = 0.02, units = dimensionless, equiv = TRACC)
- Coefficient for turbulent atmosphere heat transfer correlation.
 (default = 0.14, units = dimensionless, equiv = CTLATA)
- Exponent for turbulent atmosphere heat transfer correlation.
 (default = 1/3, units = dimensionless, equiv = ETLATA)
- (5) Coefficient for laminar atmosphere heat transfer correlation.
 (default = 0.54, units = dimensionless, equiv = CTLALA)
- (6) Exponent for laminar atmosphere heat transfer correlation. (default = 1/4, units = dimensionless, equiv = ETLALA)
- (7) Coefficient for turbulent pool heat transfer correlation.
 (default = 0.25, units = dimensionless, equiv = CTLATP)
- (8) Exponent for turbulent pool heat transfer correlation. (default = 1/4, units = dimensionless, equiv = ETLATP)
- (9) Coefficient for laminar pool heat transfer correlation.
 (default = 0.25, units = dimensionless, equiv = CTLALP)
- (10) Exponent for laminar pool heat transfer correlation. (default = 1/4, units = dimensionless, equiv = ETLALP)

- (11) Maximum void fraction permitted in a control volume pool (enforcement is approximate)
 (default = 0.4, units = dimensionless, equiv = ALPMAX)
- (12) Maximum fraction of atmospheric water vapor permitted to condense during a (subcycle) timestep.
 (default = 0.9, units = dimensionless, equiv = CFRMAX)

4408 - Pressure Iteration Parameters

Several submodels in the flow solution may be turned off if the user so desires. This capability is intended primarily for use in debugging by the code developers. The first element of the sensitivity coefficient array, C4408(1), entered as a single real number, is interpreted as five packed decimal digits, each controlling a single model. Setting any digit $\neq 0$ disables the corresponding model. Any or all of the digits may be nonzero as desired.

Setting the 100,000's digit \neq 0 disables the implicit treatment of bubble separation from two-phase pools. The resulting explicit calculation is similar (but not identical) to the model used in previous MELCOR versions through 1.8.2.

Setting the 10,000's digit \neq 0 disables the limitation on void fraction by depletion of the atmosphere.

Setting the 1,000's digit \neq 0 disables the redefinition of "old" velocities to preserve the "old" volume flow as the void fraction changes during the iteration.

Setting the 100's digit ≠ 0 disables the calculation of momentum exchange between pool and atmosphere sharing a flow path.

Setting the 10's digit \neq 0 results in using pressures at the nominal junction elevation, rather than at the average elevation of a phase in the junction opening, in the acceleration term in the momentum equation.

Setting the 1's digit \neq 0 eliminates calculation of the implicit contributions to the head terms in the momentum equation.

- Submodel flags, controlling submodels in the flow solution.
 (default = 0., units = dimensionless, equiv = XOPTN)
- A parameter used to allow the subcycle timestep to be increased whenever the convergence of velocities is much tighter than required by tolerances specified by sensitivity coefficient array 4401.
 (default = 0.005, units = dimensionless, equiv = XXCONV)

4409 – Limits and Tolerances for Time-Specified Volumes

Certain limits are placed on values input from functions or tables to define the properties of time-specified volumes. If a pool is present, it must also be between the freezing point and the critical point. In addition, discrepancies greater than roundoff are tolerated in the consistency of input, to allow for such things as imprecise interpolation in coarse tables. Of particular concern is the need to be able to specify a saturated state when *both* temperature and pressure are input. Values outside these limits and/or tolerances will result in failure to create a restart file in MELGEN or in termination of the calculation in MELCOR.

- (1) Minimum temperature. (default = 1.0, units = K, equiv = TMIN)
- (2) Maximum temperature.(default = 1.0E4, units = K, equiv = TMAX)
- (3) Minimum volume pressure. (default = 1.0, units = Pa, equiv = PMIN)
- (4) Maximum volume pressure. (default = 1.0E8, units = Pa, equiv = PMAX)
- (5) Tolerance on sum of NCG mole fractions compared to 1.0.
 (default = 0.001, units = dimensionless, equiv = TOLMFR)
- Tolerance on saturation temperature, within which input corresponding to a superheated pool or a subcooled atmosphere will be treated as saturated.
 (default = 1.0, units = K, equiv = TOLTS)

4410 – Vapor Velocity Enhancement during Direct Containment Heating

The largely parametric treatment of High Pressure Melt Ejection (HPME) in the Fuel Dispersal Interactions (FDI) package does not model coupling between the velocity of airborne debris and that of the volume atmosphere. One potentially important effect of the neglected coupling would be to increase the local gas velocities and therefore to enhance heat transfer from the atmosphere to structures in the volume. These coefficients (used only in volumes where HPME is occurring) allow a parametric treatment of the enhancement through modification of the velocities that will be used in evaluating heat transfer coefficients.

- Enhancement factor applied to volume-averaged vapor velocities during direct containment heating.
 (default = 1.0, units = dimensionless, equiv = VMULT)
- Minimum temperature of airborne debris for application of the enhancement.
 (default = 1500., units = K, equiv = TDBMIN)

4411 – Limits and Tolerances for Iterations in the CVT Package

These coefficients are used to control the iterative calculations in evaluation of the mixed-material equation of state in the CVT package.

- Tolerance (relative) in determination of the temperature, given the density and the specific internal energy.
 (default = 1.0E-6, units = dimensionless, equiv = TOLTR)
- Tolerance (relative) in matching the pressures of the pool and the atmosphere in a control volume. (The volume pressure is returned as a compressibility-weighted average of the two.)
 (default = 2.0E-5, units = dimensionless, equiv = TOLPR)
- Tolerance (absolute) in matching the pressure of a subcooled pool to that of the atmosphere in a control volume. The alternate tolerance is made necessary by the near incompressibility of liquid water. The default value is slightly greater than the pressure change associated with roundoff in liquid density at atmospheric pressure on a 32-bit computer, and represents the limit in precision with which the pressure of a subcooled liquid can be determined from its density. Because the volume pressure is returned as a compressibility-weighted average of pool and atmosphere pressures, the effect on final pressure is greatly reduced if the volume contains a significant volume of atmosphere.

 (default = 300.0, units = Pa, equiv = TOLPA)
- Minimum volume fraction to be assigned to the pool or the atmosphere in a control volume after thermodynamic calculation have been completed. Although MELCOR 1.8.2 used a (hard-wired) value of 1.0E-6, a nonzero value will result in inconsistent properties for a very small pool or atmosphere and interfere with convergence of iterations. This coefficient is provided to allow return to the older model, should the need arise. (default = 0.0, units = dimensionless, equiv = VPHMIN)

4412 – Limits and Tolerances for Iterations in the CVH Package

These coefficients are used to control the iterative calculations in solution of the hydrodynamic equations in the CVH package.

- Permitted discrepancy between the implicitly projected value and the final (1) value of the pool void fraction in any volume during solution of the implicit flow equations. (default = 0.01, units = dimensionless, equiv = ALPTOL)

4413 – Flow Blockage Friction Parameters

These parameters are used to calculate the friction loss in a flow path that has been at least partially blocked by debris. The pressure drop will be based on a generalized Ergun equation in the form

$$K_{\text{eff}} = \left[\text{C4413(1)} + \text{C4413(2)} \left(\frac{1 - \varepsilon}{\text{Re}} \right) + \text{C4413(3)} \left(\frac{1 - \varepsilon}{\text{Re}} \right)^{\text{C4413(4)}} \right] \frac{\left(1 - \varepsilon \right) L}{\varepsilon D}$$

where \mathcal{E} is the porosity, L is the path length, D is the particle diameter, and $Re = \rho i D / \mu$ is the Reynolds number based on the superficial velocity (volumetric flux) j, the fluid viscosity μ , and the particle diameter.

- (1) - Coefficient of turbulent term in generalized Ergun equation. (default = 3.5, units = dimensionless, equiv = CTERG)
- (2) - Coefficient of laminar term in generalized Ergun equation. (default = 300.0, units = dimensionless, equiv = CLERG)
- Coefficient of Achenbach term in generalized Ergun equation. (3) (default = 0.0, units = dimensionless, equiv = CCACH)
- (4) - Exponent in Achenbach term in generalized Ergun equation. (default = 0.4, units = dimensionless, equiv = CPACH)
- (5) - Minimum porosity to be used in evaluating the correlation, imposed as a bound before K_{eff} is evaluated. (default = 1.0E-6, units = dimensionless, equiv = PORMIN)

4414 – Minimum Hydrodynamic Volume Fraction

This parameter defines a fraction of the initial hydrodynamic volume in a control volume (as specified on CVHnnnBk records) that will be considered as available to hydrodynamic materials, regardless of virtual volume changes resulting from relocation of nonhydrodynamic materials such as core debris.

 Minimum fraction of the initial volume in a control volume that will always be available to hydrodynamic materials.
 (default = 1.0E-4, units = dimensionless, equiv = FVMIN)

4. Plot Variables and Control Function Arguments

The variables in the control volume hydrodynamics package that may be used for plot variables and control function arguments are listed and described below. Within slashes (//) a 'p' indicates a plot variable and a 'c' indicates a control function argument.

CVH-CLIQLEV.n	/cp/	Collapsed liquid elevation in control volume n. (units = m)
CVH-CPUT	/p/	Total CPU usage by the RUN (time-advancement) portion of CVH package. (units = s)
CVH-CPUE	/p/	CPU usage for edit in RUN portion of CVH package. (units = s)
CVH-CPUC	/p/	CPU usage for calculations in RUN portion of the CVH package. (units = s)
CVH-CPUR	/p/	CPU usage to process restart file in RUN portion of CVH package. (units = s)
CVH-E.n	/p/	Specific internal energy in control volume n. (units = J/kg)
CVH-E.m.n	/cp/	Specific internal energy of material m in control volume n. (units = J/kg)
CVH-ECV.n	/p/	Total internal energy in control volume n. (units = J)
CVH-ECV.m.n	/p/	Total internal energy of material m in control volume n. (units = J)
CVH-H.n	/cp/	Specific enthalpy in control volume n. (units = J/kg)

CVH-H.m.n	/cp/	Specific enthalpy of material m in control volume n. (units = J/kg)	
CVH-LIQLEV.n	/cp/	Swollen liquid elevation in control volume n. (units = m)	
CVH-MASS.n	/p/	Mass of material in control volume n. (units = kg)	
CVH-MASS.m.n	/cp/	Mass of material m in control volume n. (units = kg)	
CVH-P.n	/cp/	Pressure of control volume n. (units = Pa)	
CVH-PPART.m.n	/cp/	Partial pressure of material m in control volume n. (units = Pa)	
CVH-PSAT(TLIQ).n	/cp/	Saturation pressure of water at pool temperature in control volume n. (units = Pa)	
CVH-PSAT(TVAP).n	/cp/	Saturation pressure of water at atmosphere temperature in control volume n. (units = Pa)	
CVH-QUALITY.n	/p/	"Quality" (non-pool, non-fog mass fraction) in control volume n. (units = dimensionless)	
CVH-RHO.n	/cp/	Net mass density of all materials in control volume n. (units = kg/m ³)	
CVH-RHO.m.n	/p/	Mass density of material m in control volume n. (units = kg/m ³)	
CVH-RHOA.n	/c/	Mass density of atmosphere in control volume n. (units = kg/m ³)	
CVH-RHOP.n	/c/	Mass density of pool in control volume n. (units = kg/m ³)	
CVH-TLIQ.n	/cp/	Pools temperature in control volume n. (units = K)	
CVH-TOT-E	/p/	Total internal energy in the control volume hydrodynamics package. (units = J)	
CVH-TOT-E.m	/p/	Total internal energy of material m in the control volume hydrodynamics package. (units = J)	

CVH-TOT-M	/p/	Total mass in the control volume hydrodynamics package. (units = kg)					
CVH-TOT-M.m	/p/	Total mass of material m in the control volume hydrodynamics package. (units = kg)					
CVH-TSAT(A).n	/cp/	Water saturation temperature at the partial pressure of water vapor in the atmosphere of control volume n. (units = K)					
CVH-SAT(P).n	/cp/	Water saturation temperature at the pressure control volume n. (units = K)					
CVH-TVAP.n	/cp/	Atmosphere temperature in control volume n. (units = K)					
CVH-VELVAPCV.n	/p/	Velocity of atmosphere in control volume n. (units = m/s)					
CVH-VELLIQCV.n	/p/	Velocity of pool in control volume n. (units = m/s)					
CVH-VIRVOVAP.n	/p/	Virtual volume in atmosphere in control volume n. (units = m ³)					
CVH-VIRVOLIQ.n	/p/	Virtual volume in pool in control volume n. (units = m ³)					
CVH-VOID.n	/p/	Void (non-pool) volume fraction in control volume n. (units = dimensionless)					
CVH-VOLFOG.n	/cp/	Volume of fog in control volume n. (units = m ³)					
CVH-VOLLIQ.n	/cp/	Swollen volume of pool (including any vapor bubbles) in control volume n. (units = m^3)					
CVH-VOLVAP.n	/cp/	Volume of gaseous atmosphere in control volume n. (units = m ³)					
CVH-X.m.n	/cp/	Mole fraction of gaseous material m (m \geq 3) in the atmosphere of control volume n. (units = dimensionless)					

5. Example Input

This section will give several examples of input to the CVH package. Anything following an asterisk is a comment.

The first example is for a control volume with user-assigned number 1, and unimaginatively name "VOLUME ONE." It uses nonequilibrium thermodynamics, specifies horizontal flow, and is part of the reactor coolant system. (The flow direction is not used by any model; designation as part of the reactor coolant system will be used, if at all, in organizing RN package output.) The volume contains 150 m³, is 10 m high with a base at 0 m, and has a constant horizontal cross-section. Its flow area, for the purposes of defining an average velocity, is 12.5 m². It is initially filled to the 9.5 m elevation with saturated liquid water at 7.0 MPa, and the remaining space is filled by saturated water vapor.

CV00100	'VOLUME	ONE' 2	2 1	*	NEQ, vert flow, RCS
CV00101	0 0			*	Pool + fog, active
CV00103	12.5			*	Flow area
CV001A0	3			*	Pool, atmos input
CV001A1	PVOL	7.0E6	ZPOL 9.5	*	See discussion
CV001B0	0.0	0.0		*	Bottom at 0 m
CV001B1	10.0	150.0		*	150 m3 total volume

The pool will be saturated because *only* its pressure is defined. The atmosphere will consist of saturated water vapor, because no additional properties are defined. If the record

```
CV001A2 TATM 650.0 * Superheated
```

is added, the atmosphere will consist of superheated water vapor at 650 K and 7.0 MPa.

Records CV00101 and CV001A0 specify default values, and could be omitted; conditions in the volume can be made time independent by replacing the former with

```
CV00101 0 -1 * Time-indep
```

A more complicated shape, with only a third of the total volume in the lower half of the volume height, will be defined if record CV110B1 is replaced by

```
CV001B1 5.0 50.0 10.0 150.0 * 50 m3 below 5 m
```

The next example defines a volume with user-assigned number 200 named "Wet Well." It uses nonequilibrium thermodynamics. Its volume is 8000 m^3 , with a constant cross-section between elevations of -25 m and -5 m. The initial pressure is 110 kPa, and the volume is filled to the -15 m elevation with subcooled water at 313 K. The atmosphere, at 323 K, has a relative humidity of 90%. The balance consists of noncondensible gases, materials 4 and 5; the mole fractions are 80% and 20%, respectively.

```
CV20000 'Wet Well' 2 1 3 * NEQ, hrz flo, wet well CV200A1 PVOL 1.1E5 ZPOL -15.0 * Pressure, pool surface CV200A3 TPOL 313.0 TATM 323.0 * Pool, atmos temps CV200A4 RHUM 0.90 * RHUM implies PH20
```

```
CV200A6 MLFR.4 0.8 MLFR.5 0.2 * Noncondensibles
CV200B1 -25.0 0.0 -5.0 8.0E3 * Volume/Altitude table
```

The partial pressure of water vapor in the atmosphere will be 0.9 of the saturation pressure (12.2 kPa) at 323 K, or 11.0 kPa. Noncondensible gases will make up the remaining 99.0 kPa of the total pressure, with partial pressures in a 4 to 1 ratio. Note that these gases must be defined by input to the NCG package. For example, the records

```
NCG001 N2 4 * Material 4 is N2
NCG010 O2 5 * Material 5 is O2
NCG025 H2 6 * Material 6 is H2
```

will define material 4 as nitrogen, material 5 as oxygen, and material 6 as hydrogen.

To add a hydrogen source to volume 200, at a constant rate of 1 kg/s and a temperature of 800 K, simply add source records and tabular function definitions such as

```
CV200C4
         MASS.6
                   101
                        2
                             * Rate from TF 101
CV200C5
         TE
                   102
                        8
                             * Temperature from TF 102
TF10100 H2-RATE
                        1.0 * 1-point table, scale by 1.0
                             * Constant value 1.0
TF10110
         0.0 1.0
                        1.0
                             * 1-point table, scale by 1.0
TF10200
         H2-TEMP
                   1
                             * Constant value 800.0
TF10210
         0.0
              800.0
```

See the TF Package Users' Guide for information on more complicated tables. Control functions could also be used. An example will be shown later.

The third example defines a time-specified volume with user assigned number 456, name "BOUNDARY." It has a volume of 10 m³, between elevations of 1 and 2 m, and is assigned to the class "miscellaneous 1" for RN accounting purposes. It contains a pool of subcooled water with pressure and temperature given by channels 3 and 5 of external data file 7, respectively. The surface elevation as a function of time is given by tabular function 12. The atmosphere temperature is given by channel 4 of the same external data file. It is saturated (or superheated); the composition of any noncondensibles present is defined by control functions 3 and 8 (perhaps to match the composition in some other control volume).

```
CV45600 BOUNDARY 2 1 7 * NEQ, horiz flow, misc 1

CV456A1 PVOL EDF.7.3 TPOL EDF.7.5 * Pool P, T from EDF 7

CV456A2 ZPOL TF.12 * Pool surf from TF 12

CV456A3 TATM EDF.7.4 * Atm T from EDF 7

CV456A4 MLFR.4 CF.3 MLFR.5 CF.8 * NCG from CFs 3 and 8

CV456B3 1.0 0.0 2.0 10.0 * Volume/altitude table
```

The various tabular and control functions and the external data file must, of course, be defined. See the TF, CF, and EDF Package Users' Guides for discussion of the required input.

The final example defines a source of subcooled water to volume 1 with properties corresponding to the water in volume 456—that is, with the pressure and temperature given by channels 3 and 5 of external data file 7, respectively. The cumulative mass to be added is given as a function of time by control function 66.

```
CV001C3 MASS.1 66 0 * Integral mass source from CF 66
CV001CB PE 88 2 * Energy rate source from CF 88

*
CF07700 POOL-RATE DER-F 1 1.0 * Construct mass rate as
CF07700 1.0 0.0 CFVALU-66 * derivative of CF 66

*
CF08800 ENERGY-RATE MULTIPLY 2 1.0 * Multiply mass rate
CF08810 1.0 0.0 CFVALU.77 * by specific h of
CF08811 1.0 0.0 CVH-H.1.456 * pool in CV 456

*
CF06600 INT-MASS-SOURCE . . * Input as appropriate
```

This input calculates the appropriate rate of enthalpy addition as control function 88. The procedure is to first differentiate the cumulative mass source, given by control function 66, to define the source rate in control function 77, and then multiply this rate by the specific enthalpy of the pool (material 1) in control volume 456. See the Control Function (CF) Package Users' Guide for more information on specific CF input.

6. CVH Package Output

Each printed edit generated by the CVH package in MELGEN and MELCOR contains a snapshot description of the state of all control volumes, with the output organized in tabular form. Many column headings are abbreviated, but most are relatively clear—particularly when it is understood that "LIQ" refers to pool and "VAP" to atmosphere. One frequent source of confusion is that, in CVH output, "VOID FRACTION" and "QUALITY" refer to the partition of volume and of water mass, respectively, between pool and atmosphere. The vapor bubble content of the pool may be inferred from the difference between the swollen liquid level, "S-Z-POOL," and the collapsed liquid level "C-Z-POOL." The edit includes a summary of the integrated sources in each control volume, and of the current partition of volume between hydrodynamic ("MATL") and virtual volume.

A description of the nodalization, including a list of all flow paths connected to each volume, will be found in the "FLOW PATH TIME INDEPENDENT DATA EDIT" generated by the FL package in MELGEN and in the first edit for each MELCOR run.

Users are strongly advised to check the initial edit generated by MELGEN—in addition to the contents of the diagnostic file (MEGDIA) —before proceeding with a calculation.

7. Diagnostics and Error Messages

Diagnostic messages may be written either by MELGEN or by MELCOR. Messages from MELGEN ordinarily report errors or inconsistencies in input; problems encountered while completing the definition of initial conditions may also be reported. If an error is encountered, no restart file will be written; errors must be corrected before MELCOR can be run.

Messages from MELCOR report problems encountered during the time advancement of a calculation. If an error is severe, the calculation will be stopped and a restart dump written corresponding to conditions at the beginning of the fatal timestep.

A user input option, CVHTRACE, turns on a detailed, step-by-step tracing of the numerical solution of the hydrodynamic equations, with information written to the diagnostic file (MELDIA). If the calculational performance of the CVH package is poor, this information may be useful in determining the cause.

If any package requires a timestep below the user-specified minimum value, the MELCOR executive will stop the calculation. (The SOFTDTMIN record in the Executive Package Users' Guide allows this treatment to be modified.) When this occurs, the executive will repeat the last attempt with CVHTRACE turned on. In most such cases, the unacceptable timestep cut will have been demanded by the CVH package; in a large fraction of these, this will be found to be a result of unacceptable boundary conditions imposed by other packages. The output from CVHTRACE is often helpful in identifying the underlying cause.

7.1 Input and Execution Messages

Messages resulting from errors in record formats or unrecognized records in user input to MELGEN include the record identifier and sufficient information to allow the user to identify the error. Typical errors include failure to supply all required input records, and incomplete specification or overspecification of the initial thermodynamic state of a control volume. Inconsistencies with MEGLEN input to other packages, including failure to correctly define any tabular or control functions or external data files required to define sources, will also be identified.

Input processing continues after an error has been found in order to identify multiple errors, but MEGLEN will not write an initial restart until all input errors have been eliminated. The default assumptions used to allow processing to continue may themselves lead to additional error messages. If one of a group of input diagnostics appears irrelevant to the

actual input, the proper strategy is to make as many corrections as possible and rerun MELGEN; the other error messages will be eliminated or clarified.

Error or warning messages may be issued during execution of MELCOR for any of a number reasons. These include attempts by another package or a CVH sink to remove more mass or energy than is contained in the associated control volume, improper relocation of virtual volume by other packages, and errors in tabular or control functions or external data files defining CVH sources or the properties of time-specified volumes. Execution will continue, with a reduced system timestep, when it makes sense to do so; the request for a system fallback will be noted.

In some cases, the thermodynamics routines will transfer energy between the pool and atmosphere of a control volume rather than return a subfreezing temperature for one of them. Such occurrences are noted; a problem with input is usually involved. A special case is the discharge of a high-pressure accumulator, where the gas temperature will fall below freezing under adiabatic expansion. Although MELCOR thermodynamics does not permit temperatures below 273.15 K, this energy transfer allows the calculation to continue with an isothermal expansion of gas after the freezing point is reached. (After fifty occurrences of such energy transfer, further warnings are suppressed.)

Coding of the CVH package includes a number of messages warning of apparent logic errors, with the text identifying them as such. The appearance of a message of this type probably involves a coding error in MELCOR; the code development team should be informed.

7.2 CVHTRACE Option

Inclusion of the CVHTRACE record in MELCOR input enables tracing of the calculations through which the CVH package advances. The result will be a large number of informative messages written to the diagnostic file (MELDIA). These messages follow very closely the description of the CVH solution algorithm outlined in the CVH/FL Reference Manual.

The volume of messages, while not nearly so large as was produced by the obsolete MELCOR DEBUG option, is large enough that it should not be used for more than a few cycles. Therefore, its activation is not recorded in the restart file; tracing is active if and only if the CVHTRACE record is present in MELCOR input for the current run.

The CVHTRACE option evolved as a partial substitute for problem debugging using system-specific debugging software such as dbx on UNIX systems. In essence, it automates the tracing and examination of variables habitually used by the code developers to investigate problems in calculations. The output assumes that the user knows a little about MELCOR numerics, but is not (intended to be) excessively cryptic.

Use of the CVHTRACE option should aid in identification of "problem areas" in a calculation. If a calculation is proceeding smoothly but with very small timesteps, the information provided by the message

NEXT TIME STEP LIMITED TO n.nnnnEeee S BY <something>

should identify the reason. If the timesteps are limited by the material Courant condition in some volume, it may be appropriate to combine this volume with a larger neighbor to ease the constraint. If the limit is the rate of change in temperature or pressure in some volume, the cause may be simply a rapid transient in conditions, after which the timestep should recover. If the system is underdamped, such a transient may persist long after the initial perturbation has passed. This may reflect input data that places too little frictional loss in flow paths. If no such transient should be occurring, the problem may be a rapidly fluctuating boundary condition imposed on that volume by some other package. It may be possible to modify input to the other package to reduce the fluctuation.

If, on the other hand, each advancement is found to involve many iterations with repeated subcycle and timestep fallbacks, it is likely that one or two volumes or flow paths will appear repeatedly in the lists of "last to converge" or "failed to converge." Attention should then be focused on these volumes and/or flow paths, and their relationships to the core, heat structures, and other elements of MELCOR modeling. Simple changes in nodalization, particularly in junction opening heights, inertial lengths, momentum exchange lengths and loss coefficients in the Flow Path input may be sufficient to eliminate the problem. Another strategy is to restrict the timestep using TIMEn records in the Executive package input to a value commensurate with the successful subcycle advancements.

If convergence problems are seen for a flow path which is ultimately found to be choked, it may be appropriate to increase the loss coefficients for that path and/or to increase the momentum exchange length to reduce the change in velocity calculated before choking is considered.

If a volume is repeatedly mentioned in association with the message

***ADVANCEMENT FAILED: THERMO ERROR

any sources or sinks in that volume, from CVH input or other packages, should be closely examined. The most common cause of such an error is a source in the volume that drives the volume out of the range of validity of the equation of state.

Throughout the process, however, the user should remain aware that CVHTRACE can only display symptoms. The underlying causes of a problem may lie in areas of the calculation which are apparently experiencing no difficulties at all.

An outline of the contents of the diagnostic file is given below, for a case where the CVHTRACE option is enabled. Four character strings in the messages should be noted as potential search patterns for the diagnostic file:

- "===" marks the start of a MELCOR timestep;
- "..." marks the start of an attempted step (full or subcycle) in CVH;
- "---" marks the successful completion of such an advancement; and
- "***" marks a problem, a point where a calculation had to be repeated, or a point where a compromise was required (for example, the user input minimum timestep overrode the value desired by CVH).

Indentation is used as a further aid to scanning the contents of the diagnostic file. This indentation is duplicated in the example messages shown below.

7.2.1 Main Advancement

The start of each MELCOR timestep is marked by the message

===CVH ADVANCEMENT FOR CYCLE nnnnnn DT = x.xxxxEeee S

If sinks (negative sources) of mass and/or energy specified by CVH input require more mass or energy than is present in one or more volumes, the problem volumes are listed, followed by the message

***FALLBACK: EXCESSIVE MASS OR ENERGY SINK

and a MELCOR fallback is performed. Tracing will begin again at "===CVH ADVANCEMENT ..." with a smaller value of DT.

The start of each attempted CVH (sub)cycle is marked by the message

...ATTEMPT (SUB)STEP OF x.xxxxEeee S, PRESSURE ITERATION n

"Pressure iteration" refers to (re)linearization of terms involving new volume pressures in the acceleration of flows, and (re)solution of the resulting flow equations.

Diagnostic messages are generated during solution of the flow equations. These are discussed below, in Section 7.2.2. If the solution fails, a fallback within CVH is executed, and tracing will generally begin again at "...ATTEMPT (SUB)STEP ..." with a smaller substep. However, if the substep has become too small, the message

***FALLBACK: SUBCYCLE STEP TOO SMALL COMPARED TO DT

is generated, a MELCOR fallback is executed. Tracing will begin again at "===CVH ADVANCEMENT ..." with a smaller value of DT.

Once the flow solution is complete, mass and energy moves are computed, the (material) Courant limit is calculated and noted as

COURANT LIMIT OF x.xxxxEee S SET BY VOLUME nnn

(A further message is provided for if this limit is exceeded, but should not appear given current coding.)

The new volume pressures are computed from the new masses and energies. If the discrepancy from the linearly-projected pressure is excessive, the offending volumes are noted, and the message

***ADVANCEMENT FAILED: PRESSURE CONVERGENCE FAILURE

is generated. Tracing begins again at "...ATTEMPT (SUB)STEP ..." either as a new pressure iteration or, if the maximum number of iterations has been reached, with a decreased substep size following an internal fallback.

If errors occur in evaluation of the equation of state, the problem volumes are noted, the message

***ADVANCEMENT FAILED: THERMO ERROR

is written, an internal fallback is executed, and tracing begins again at "...ATTEMPT (SUB)STEP ..." with a decreased substep size.

Messages are coded for a possible "water pack fix-up", but this is not enabled in current versions of MELCOR.

When a (sub)step is completed successfully, the net advancement to that point is noted as

---ADVANCEMENT SUCCESSFUL THROUGH x.xxxxEeeee S

The possibility of choking is then evaluated. If it is detected, the step is repeated with the message

***REPEAT FOR CHOKING IN FLOW PATHS nnn nnn ...

When the advancement reaches the end of the MELCOR timestep, the net changes during the step are examined and, if all are acceptable, a proposed new timestep is estimated. This is noted as

NEXT TIME STEP LIMITED TO n.nnnnEee S BY <something>

where "<something>" may be a change in pressure or temperature (using limits defined by Sensitivity Coefficients in array 4400) in some volume (the volume number will be noted), the Courant limit (the relevant volume number has already been noted), or the estimated accuracy of some solution procedure. This will be followed by the message

***MINIMUM TIMESTEP OVERRIDES LIMIT

if appropriate.

If some change is excessive (again based on Sensitivity Coefficients in array 4400), however, a message is issued:

***EXCESSIVE CHANGE IN <something>, VOLUME nnn

where "<something>" may be POOL TEMPERATURE, ATMOSPHERE TEMPERATURE, or PRESSURE. It will generally be followed by the message

***FALLBACK: CHANGE DURING TIMESTEP TOO GREAT

and the entire MELCOR step will be repeated with a decreased value of DT. However, if the step is already within a factor of 2 of the minimum, the calculation will continue with the warning message

***MINIMUM TIMESTEP PREVENTS FALLBACK

7.2.2 Flow Solution

Solution of the flow equation is iterative, because donor properties and friction terms are nonlinear functions of the flow velocities. When the iteration converges, the message

VELOCITIES CONVERGED IN CVHMOM ON ITERATION nn

is written. If iteration was required, this is followed by either or both of the messages

LAST VELOCITIES TO REVERSE INCLUDE nnnc nnnc <etc>
LAST VELOCITIES TO CONVERGE INCLUDE nnnc nnnc <etc>

where nnn is a flow path number and c is P for pool or A for atmosphere. If the number of flows in either list exceeds 10, the list is truncated. "Reversal" is with respect to the previous iteration (so that donoring must be switched). "Convergence" requires a change in magnitude from the previous iteration within the limits set by Sensitivity Coefficients in array 4401.

In some cases, the volumetric flows converge even though the velocities do not, because of iteration-to-iteration changes in the flow-path void fraction. If this is the case, the messages will be

VOLUME FLOWS CONVERGED IN CVHMOM ON ITERATION nn UNCONVERGED VELOCITIES INCLUDE nnnc nnnc <etc>

If, after a number of iterations defined by a Sensitivity Coefficient in array 4401, neither velocities nor flows have converged, but the unconverged ones do not contribute significantly to the projected new pressure, the iteration is terminated with the message

PRESSURES CONVERGED IN CVHMOM ON ITERATION nn

and either or both of the messages

REVERSED VELOCITIES INCLUDE nnnc nnnc <etc>
UNCONVERGED VELOCITIES INCLUDE nnnc nnnc <etc>

(The default is not to allow acceptance of a velocity solution on this basis.)

The solution may fail, with either the message

***VELOCITY ITERATION FAILED IN CVHMOM

or the message

***FLOW MATRIX IN CVHMOM 'SINGULAR' ON ITERATION nn

The maximum number of iterations is set by a Sensitivity Coefficient in array 4401.